

# ***STIC Search Report***

***EIC 1700***

**STIC Database Tracking Number: 191442**

**TO: Ben Sackey  
Location: REM 5B31  
Art Unit : 1626  
June 2, 2006**

**Case Serial Number: 10/727644**

**From: Kathleen Fuller  
Location: EIC 1700  
REMSEN 4B28  
Phone: 571/272-2505  
Kathleen.Fuller@uspto.gov**

## **Search Notes**

## SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: BEN SACKG Examiner #: 73489 Date: 5/30/06  
 Art Unit: 1626 Phone Number 302-207-004 Serial Number: 10/727, 644  
 Mail Box and Bldg/Room Location: REM 553 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

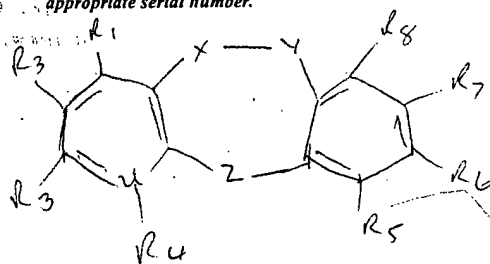
\*\*\*\*\*

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Triyclic fused heterocycle Compds, Process for Prep. and use thereof  
 Inventors (please provide full names): Shuji Jinno et al.

Earliest Priority Filing Date: 6/03/99

\*For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.



wherein 2 is -O- or -S-  
 $R^1 - R^8$  are as defined

2 is -C-

X and Y are a bond or when  $X - Y$  is  $CH_2CH_2$ ,  $CH_2CH_2$ ,  $CH_2O$ ,  $CH_2CO$ ,  $CH=CH$ ,  $CH=COCH_3$  or  $CH=COCH_3$  and  $R^1 - R^8$  is an aromatic ring, a substituted aromatic ring, a heterocycle etc

Thanks

## STAFF USE ONLY

	Type of Search	Vendors and cost where applicable
Searcher: <u>R. Fuller</u>	NA Sequence (#) _____	STN <input checked="" type="checkbox"/> _____
Searcher Phone #: _____	AA Sequence (#) _____	Dialog _____
Searcher Location: _____	Structure (#) <u>2</u>	Questel/Orbit _____
Date Searcher Picked Up: _____	Bibliographic _____	Dr. Link _____
Date Completed: <u>6/2/06</u>	Litigation _____	Lexis/Nexis _____
Searcher Prep & Review Time: <u>40</u>	Fulltext _____	Sequence Systems _____
Clerical Prep Time: _____	Patent Family _____	WWW/Internet _____
Online Time: <u>48</u>	Other _____	Other (specify) _____

=> FILE REG

FILE 'REGISTRY' ENTERED AT 11:03:05 ON 02 JUN 2006  
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Property values tagged with IC are from the ZIC/VINITI data file  
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STRUCTURE FILE UPDATES: 1 JUN 2006 HIGHEST RN 886490-27-3  
DICTIONARY FILE UPDATES: 1 JUN 2006 HIGHEST RN 886490-27-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

\*\*\*\*\*  
\*  
\* The CA roles and document type information have been removed from \*  
\* the IDE default display format and the ED field has been added, \*  
\* effective March 20, 2005. A new display format, IDERL, is now \*  
\* available and contains the CA role and document type information. \*  
\*  
\*\*\*\*\*

Structure search iteration limits have been increased. See HELP SLIMITS  
for details.

REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=> FILE HCAPL

FILE 'HCAPLUS' ENTERED AT 11:03:09 ON 02 JUN 2006  
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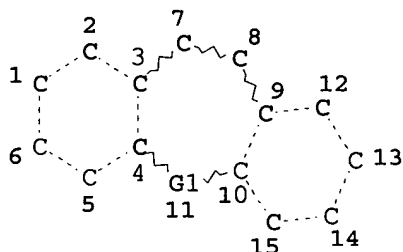
FILE COVERS 1907 - 2 Jun 2006 VOL 144 ISS 24  
FILE LAST UPDATED: 1 Jun 2006 (20060601/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> D QUE L26

L11 STR



*6,541 structures from query*

VAR G1=O/S

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE

L14 6541 SEA FILE=REGISTRY SSS FUL L11

L16 1855 SEA FILE=HCAPLUS ABB=ON L14

L17 703 SEA FILE=HCAPLUS ABB=ON L16 (L) PREP/RL

L18 661 SEA FILE=HCAPLUS ABB=ON L17 AND (1840-1999)/PRY,AY,PY

L19 26 SEA FILE=HCAPLUS ABB=ON L16 AND ?ASTHM?

L20 21 SEA FILE=HCAPLUS ABB=ON L16 AND RESPIRA?

L21 38 SEA FILE=HCAPLUS ABB=ON L19 OR L20

L26 9 SEA FILE=HCAPLUS ABB=ON L21 AND L18

*had to limit by utility because 661 CA references limited by date*

=> SEL HIT RN L26 1-9

E1 THROUGH E370 ASSIGNED

=> D L26 1-9 BIB ABS HITIND FHITSTR

*did only 1 structure per CA references as there are 320 structures in the 9 CA refs*

L26 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

AN 2000:881137 HCAPLUS

DN 134:29329

TI Preparation of tricyclic fused heterocycle compounds as **antiasthmatics** and **respiratory** tract hypersensitiveness inhibitors

IN Jinno, Shuji; Okita, Takaaki; Ohtsuka, Naomi; Yamashita, Shinya; Hata, Junichiro; Takeo, Jiro

PA Nippon Suisan Kaisha, Ltd., Japan

SO PCT Int. Appl., 136 pp.

CODEN: PIXXD2

DT Patent

LA Japanese

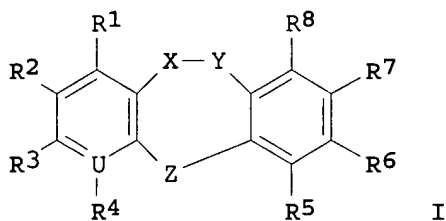
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000075127	A1	20001214	WO 2000-JP3592	20000602 <--
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU,				

*applicant*

ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU,  
 LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD,  
 SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU,  
 ZA, ZW  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,  
 DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,  
 CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

CA 2370013	AA	20001214	CA 2000-2370013	20000602 <--
EP 1182200	A1	20020227	EP 2000-935528	20000602 <--
EP 1182200	B1	20050831		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, MC, PT, IE, SI, LT, LV, FI, RO				
BR 2000011529	A	20021217	BR 2000-11529	20000602 <--
RU 2211837	C2	20030910	RU 2001-132596	20000602 <--
NZ 515666	A	20031031	NZ 2000-515666	20000602 <--
JP 3471778	B2	20031202	JP 2001-502410	20000602 <--
AU 777414	B2	20041014	AU 2000-51044	20000602 <--
AT 303376	E	20050915	AT 2000-935528	20000602 <--
ES 2248080	T3	20060316	ES 2000-935528	20000602 <--
ZA 2001009565	A	20030411	ZA 2001-9565	20011120 <--
NO 2001005832	A	20020201	NO 2001-5832	20011129 <--
BG 106169	A	20020531	BG 2001-106169	20011203 <--
US 6602898	B1	20030805	US 2002-980581	20020226 <--
US 2003220360	A1	20031127	US 2002-291429	20021112 <--
US 6700013	B2	20040302		
JP 2004083567	A2	20040318	JP 2003-173495	20030618 <--
US 2004127713	A1	20040701	US 2003-727644	20031205 <--
PRAI JP 1999-157181	A	19990603	<--	
JP 2001-502410	A3	20000602		
WO 2000-JP3592	W	20000602		
US 2002-980581	A3	20020226		
US 2002-291429	A1	20021112		
OS MARPAT 134:29329				
GI				



- AB The title compds. I [X is CH, CH<sub>2</sub>, CHR, etc. (wherein R is lower alkyl or substituted lower alkyl); Y is CH, CH<sub>2</sub>, or CO; Z is O, S, SO, or SO<sub>2</sub>; U is C or N; R<sub>1</sub> to R<sub>4</sub> are each independently hydrogen, OR, SR (wherein R is as defined above), an aromatic ring, a heterocycle, or the like; and R<sub>5</sub> to R<sub>8</sub> are each independently hydrogen, alkyl, etc; at least one of R<sub>5</sub> to R<sub>8</sub> is OH] are prepared The compds. exhibit excellent pharmacol. activities such as relaxation of tracheal smooth muscle, suppression of **respiratory** tract hypersensitiveness, etc. 11-Ethyl-7,9-dihydroxy-10,11-dihydrodibenzo[b,f]thiepin-10-one at 30 mg/kg orally gave significant inhibition of **respiratory** tract hypersensitiveness in guinea pigs.
- IC ICM C07D313-14  
 ICS C07D337-14; C07D405-04; C07D407-04; C07D409-04; C07D491-06;

A61K031-31; A61K031-335; A61K031-343; A61K031-38; A61K031-381;  
A61K031-4353; A61K031-4427; A61P011-06; A61P011-08; A61P029-00

CC 27-21 (Heterocyclic Compounds (One Hetero Atom))  
Section cross-reference(s): 1

ST tricyclic fused heterocycle prepn **antiasthmatic**;  
**respiratory** tract hypersensitiveness inhibitor tricyclic fused  
heterocycle

IT **Respiratory tract**  
(hypersensitiveness; preparation of tricyclic fused heterocycle compds. as  
**antiasthmatics** and **respiratory tract**  
hypersensitiveness inhibitors)

IT Phagocyte  
(infiltration; preparation and effect of tricyclic fused heterocycle compds.  
on phagocytic infiltration into **respiratory tract**.)

IT Toxicity  
(preparation and toxicity of tricyclic fused heterocycle compds. with effect  
on **asthma** and **respiratory tract** hypersensitiveness)

IT 312300-98-4P 312300-99-5P 312301-00-1P  
312301-01-2P 312301-02-3P 312301-03-4P  
312301-04-5P 312301-05-6P 312301-06-7P  
312301-07-8P 312301-08-9P 312301-09-0P  
312301-10-3P 312301-11-4P 312301-12-5P  
312301-13-6P 312301-14-7P 312301-15-8P  
312301-16-9P 312301-17-0P 312301-18-1P  
312301-19-2P 312301-20-5P 312301-21-6P  
312301-22-7P 312301-23-8P 312301-24-9P  
312301-25-0P 312301-26-1P 312301-27-2P  
312301-28-3P 312301-29-4P 312301-30-7P  
312301-31-8P 312301-32-9P 312301-33-0P  
312301-34-1P 312301-35-2P 312301-36-3P  
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312302-76-4P 312302-77-5P 312302-78-6P  
312302-79-7P 312302-80-0P 312302-81-1P  
312302-82-2P 312302-83-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; **USES (Uses)**

(preparation of tricyclic fused heterocycle compds. as  
**antiasthmatics** and **respiratory tract**  
hypersensitiveness inhibitors)

IT 50-30-6 75-03-6, Ethyl iodide 79-03-8, Propionyl chloride 91-16-7  
98-80-6, Phenylboronic acid 99-60-5 140-89-6, Potassium xanthogenate  
143-33-9, Sodium cyanide 147-93-3 500-99-2 693-02-7, 1-Hexyne  
700-96-9 2859-78-1 5470-11-1, Hydroxylamine hydrochloride 10272-07-8  
19472-74-3 21085-72-3, Methyl acetobromoglucuronate 21739-92-4  
30481-27-7 51546-12-4 54663-78-4, 2-(Tributylstannyl)thiophene  
145343-76-6 193199-01-8 312303-26-7  
312303-27-8 312303-28-9 312303-29-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of tricyclic fused heterocycle compds. as  
**antiasthmatics** and **respiratory tract**  
hypersensitiveness inhibitors)

IT 2457-76-3P 19689-66-8P 59748-90-2P 66086-38-2P 127905-36-6P  
193199-25-6P 193200-15-6P 212626-86-3P 219696-68-1P  
312302-85-5P 312302-86-6P 312302-87-7P 312302-88-8P 312302-89-9P  
312302-90-2P 312302-91-3P 312302-92-4P 312302-93-5P  
312302-94-6P 312302-95-7P 312302-96-8P 312302-97-9P  
312302-98-0P 312302-99-1P 312303-00-7P 312303-01-8P  
312303-02-9P 312303-03-0P 312303-04-1P 312303-05-2P  
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312303-13-2P 312303-14-3P 312303-15-4P 312303-16-5P  
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312303-21-2P 312303-22-3P 312303-23-4P 312303-24-5P  
312303-25-6P 312303-30-3P 312303-31-4P 312303-32-5P 312303-33-6P  
312303-34-7P 312303-35-8P 312303-36-9P

RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)

(preparation of tricyclic fused heterocycle compds. as  
**antiasthmatics** and **respiratory tract**  
hypersensitiveness inhibitors)

IT 312300-98-4P

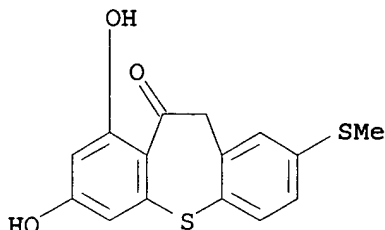
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); **PREP (Preparation)**; THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; **USES (Uses)**

(preparation of tricyclic fused heterocycle compds. as  
**antiasthmatics** and **respiratory tract**

hypersensitiveness inhibitors)

RN 312300-98-4 HCAPLUS

CN Dibenzo[b,f]thiepin-10(11H)-one, 7,9-dihydroxy-2-(methylthio)- (9CI) (CA INDEX NAME)



RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

AN 1997:145245 HCAPLUS

DN 126:157408

TI Preparation of N-(arylcarbonyl or heterocyclylcarbonyl)amino(carboxyalkenyl)bicycloheptane derivatives or analogs thereof and prostaglandin D2 (PGD2) antagonists containing the same

IN Ohtani, Mitsuaki; Arimura, Akinori; Tsuru, Tatsuo; Kishino, Junji; Honma, Tsunetoshi

PA Shionogi and Co., Ltd., Japan

SO PCT Int. Appl., 242 pp.

CODEN: PIXXD2

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9700853	A1	19970109	WO 1996-JP1685	19960619 <--
	W: AL, AU, BB, BG, BR, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KR, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	CA 2225250	AA	19970109	CA 1996-2225250	19960619 <--
	CA 2225250	C	20050322		
	AU 9661370	A1	19970122	AU 1996-61370	19960619 <--
	AU 714312	B2	19991223		
	EP 837052	A1	19980422	EP 1996-918841	19960619 <--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI				
	CN 1193315	A	19980916	CN 1996-196326	19960619 <--
	CN 1134410	B	20040114		
	BR 9608498	A	19990706	BR 1996-8498	19960619 <--
	CZ 285870	B6	19991117	CZ 1997-4013	19960619 <--
	JP 3195361	B2	20010806	JP 1997-503724	19960619 <--
	TW 513422	B	20021211	TW 1996-85107425	19960619 <--
	PL 185107	B1	20030228	PL 1996-324115	19960619 <--
	NO 9705994	A	19980223	NO 1997-5994	19971219 <--
	US 6172113	B1	20010109	US 1998-973983	19980422 <--
	US 6384075	B1	20020507	US 2000-506608	20000218 <--
	US 6498190	B1	20021224	US 2000-506606	20000218 <--



	JP 2001288160	A2	20011016	JP 2001-73708	20010315 <--
	JP 3701878	B2	20051005		
PRAI	JP 1995-154575	A	19950621	<--	
	JP 1997-503724	A3	19960619	<--	
	WO 1996-JP1685	W	19960619	<--	
	US 1998-973983	A3	19980422	<--	

OS MARPAT 126:157408

GI For diagram(s), see printed CA Issue.

AB Comps. of general formula [I; ring Y = Q - Q3; A = alkylene optionally interrupted with phenylene or hetero atoms and optionally containing oxo and/or unsatd. bonds; B = H, alkyl, aralkyl, acyl; R = CO2R1, CH2OR2, CONR3R4; R1, R2 = H, alkyl; R3, R4 = H, alkyl, OH, alkylsulfonyl; X1 = single bond, phenylene, naphthylene, thiophenediyl, indolediyl, oxazolediyl; X2 = single bond, N:N, N:CH, CH:N, CH:NN, CH:NO, C:NNHCSNH, C:NNHCONH, CH:CH, CH(OH), CCl:CCl, (CH2)n, C.tplbond.C, NR5, NR5CO, NR5SO2, NR5CONR5, CONR5, SO2NR5, O, S, SO, SO2, CO, oxadiazolediyl, thiadiazolediyl, tetrazolediyl; wherein R5 = H, alkyl; X3 = alkyl, alkenyl, alkynyl, aryl, aralkyl, heterocyclyl, cycloalkyl, cycloalkenyl, thiazolylidene, etc.; Z = SO2, CO; m = 0,1; wherein if the substituents are in the form of rings, they may be optionally substituted] or salts thereof or hydrates thereof are prepared These comps. are useful as a PGD2 antagonists and thus usable in, for example, a remedy for systemic mastocytosis or systemic mast cell activation disorders, a drug for bronchoconstriction, an **asthmatic**, a drug for allergic rhinitis agent, a drug for allergic conjunctivitis, a drug for urticaria, a remedy for ischemia reperfusion disorders or an antiinflammatory agent. They are particularly useful in the treatment of nasal occlusion. Thus, a bicyclo[2.2.1]heptane derivative (II; R = Me, R7 = H) was condensed with 2-chlorosulfonyldibenzofuran in the presence of Et3N in CH2Cl2 to give, after saponification, II .Na (R = H, R7 = Q3). I in vitro inhibited the

binding

of [3H]PGD2 to PGD2 receptor preparation from human blood platelet fraction with IC50 of 0.003-8.6 µM. A tablet and granule formulation containing the title compound (III.1/2Ca) were described.

IC ICM C07C233-52

ICS C07C233-84; C07C271-24; C07C311-06; C07C311-11; C07C311-13;  
C07C311-19; C07D493-08; C07D495-08; A61K031-16; A61K031-18;  
A61K031-27; A61K031-33; A61K031-34; A61K031-35; A61K031-38

CC 27-21 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 1, 25, 28, 63

ST aminobicycloheptane prepn prostaglandin D2 antagonist; PGD2 antagonist;  
aminocarboxyalkenylbicycloheptane prepn antiinflammatory; systemic  
mastocytosis treatment dibenzofurancarboxylaminobicycloheptane; mast cell  
activation disorder treatment aminobicycloheptane; bronchoconstriction  
treatment aminobicycloheptane; **asthmatic** treatment  
aminobicycloheptane; allergic rhinitis treatment aminobicycloheptane;  
conjunctivitis allergic treatment aminobicycloheptane; urticaria remedy  
treatment aminobicycloheptane; ischemia reperfusion disorder treatment  
aminobicycloheptane; nasal occlusion treatment aminobicycloheptane

IT Anti-inflammatory agents

**Antiasthmatics**

Bronchodilators

Urticaria

(preparation of amino(carboxyalkenyl)bicycloheptane derivs. as prostaglandin  
D2 antagonists for disease therapy)

IT	132747-47-8P	142646-81-9P	186528-33-6P	186528-34-7P	186528-35-8P
	186528-36-9P	186528-37-0P	186528-38-1P	186528-39-2P	186528-41-6P
	186528-42-7P	186528-43-8P	186528-44-9P	186528-45-0P	186528-46-1P
	186528-47-2P	186528-48-3P	186528-49-4P	186528-50-7P	186528-51-8P
	186528-52-9P	186528-53-0P	186528-54-1P	186528-55-2P	186528-56-3P

186528-57-4P	186528-58-5P	186528-59-6P	186528-60-9P	186528-61-0P
186528-62-1P	186528-63-2P	186528-64-3P	186528-65-4P	186528-66-5P
186528-67-6P	186528-68-7P	186528-69-8P	186528-70-1P	186528-71-2P
186528-72-3P	186528-73-4P	186528-74-5P	186528-75-6P	186528-76-7P
186528-77-8P	186528-78-9P	186528-79-0P	186528-80-3P	186528-81-4P
186528-82-5P	186528-83-6P	186528-84-7P	186528-85-8P	186528-86-9P
186528-87-0P	186528-88-1P	186528-89-2P	186528-90-5P	186528-91-6P
186528-92-7P	186528-93-8P	186528-94-9P	186528-95-0P	186528-96-1P
186528-97-2P	186528-98-3P	186529-00-0P	186529-02-2P	186529-03-3P
186529-04-4P	186529-06-6P	186529-07-7P	186529-08-8P	186529-09-9P
186529-10-2P	186529-11-3P	186529-12-4P	186529-13-5P	186529-14-6P
186529-15-7P	186529-16-8P	186529-17-9P	186529-18-0P	186529-19-1P
186529-20-4P	186529-21-5P	186529-22-6P	186529-23-7P	186529-24-8P
186529-25-9P	186529-27-1P	186529-29-3P	186529-31-7P	186529-33-9P
186529-34-0P	186529-35-1P	186529-37-3P	186529-38-4P	186529-39-5P
186529-40-8P	186529-41-9P	186529-42-0P	186529-43-1P	186529-44-2P
186529-45-3P	186529-46-4P	186529-47-5P	186529-48-6P	186529-49-7P
186529-50-0P	186529-51-1P	186529-52-2P	186529-53-3P	186529-54-4P
186529-55-5P	186529-56-6P	186529-57-7P	186529-58-8P	186529-59-9P
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186529-73-7P	186529-76-0P	186529-80-6P	186529-83-9P	186529-84-0P
186529-85-1P	186529-86-2P	186529-87-3P	186529-88-4P	186529-89-5P
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186529-95-3P	186529-96-4P	186529-97-5P	186529-98-6P	186529-99-7P
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186530-57-4P	186530-58-5P	186530-59-6P	186530-60-9P	

186530-61-0P 186530-62-1P 186530-63-2P

186530-64-3P	186530-65-4P	186530-66-5P	186530-67-6P	
186530-68-7P	186530-69-8P	186530-70-1P	186530-71-2P	186530-72-3P
186530-73-4P	186530-74-5P	186530-75-6P	186530-76-7P	186530-77-8P
186530-78-9P	186530-79-0P	186530-80-3P	186530-81-4P	186530-82-5P
186530-83-6P	186530-84-7P	186530-85-8P	186530-86-9P	186530-87-0P
186530-88-1P	186530-89-2P	186530-90-5P	186530-91-6P	186530-92-7P
186530-93-8P	186530-94-9P	186530-95-0P	186530-96-1P	186530-97-2P
186530-98-3P	186530-99-4P	186531-00-0P	186531-01-1P	186531-02-2P
186531-03-3P	186531-04-4P			

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)

(preparation of amino(carboxyalkenyl)bicycloheptane derivs. as prostaglandin D2 antagonists for disease therapy)

IT	186533-63-1P	186533-64-2P	186533-65-3P	186533-66-4P	186533-67-5P
	186533-68-6P	186533-69-7P	186533-70-0P	186533-71-1P	186533-72-2P
	186533-73-3P	186533-74-4P	186533-75-5P	186533-76-6P	
	186533-77-7P	186533-78-8P	186533-79-9P		
	186533-80-2P	186533-81-3P	186533-82-4P	186533-83-5P	186533-84-6P
	186533-85-7P	186533-86-8P	186533-87-9P	186533-88-0P	186533-89-1P
	186533-90-4P	186533-91-5P	186533-93-7P	186533-94-8P	186533-95-9P
	186533-96-0P	186533-97-1P	186533-98-2P	186533-99-3P	186534-00-9P
	186535-60-4P	186535-61-5P	186536-04-9P	186536-06-1P	186536-08-3P
	186536-10-7P	186536-12-9P	186536-14-1P	186536-18-5P	186536-20-9P
	186536-23-2P	186536-25-4P	186744-64-9P	186745-86-8P	186749-85-9P
	186749-86-0P	186749-88-2P			

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)  
(preparation of amino(carboxyalkenyl)bicycloheptane derivs. as prostaglandin D2 antagonists for disease therapy)

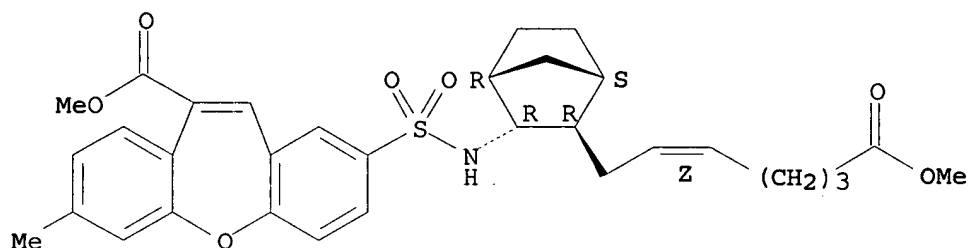
IT 186530-59-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)  
(preparation of amino(carboxyalkenyl)bicycloheptane derivs. as prostaglandin D2 antagonists for disease therapy)

RN 186530-59-6 HCAPLUS

CN Dibenz[b,f]oxepin-10-carboxylic acid, 2-[[[3-(7-methoxy-7-oxo-2-heptenyl)bicyclo[2.2.1]hept-2-yl]amino]sulfonyl]-7-methyl-, methyl ester, [1R-[1 $\alpha$ ,2 $\beta$ ,3 $\alpha$ (Z),4 $\alpha$ ]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



L26 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

AN 1991:632258 HCAPLUS

DN 115:232258

TI Preparation of dibenzoheterocyclic hydroxamic acids and -hydroxy ureas as 5-lipoxygenase inhibitors

IN Girard, Yves; Hamel, Pierre; Delorme, Daniel

PA Merck and Co., Inc., USA

SO U.S., 14 pp.

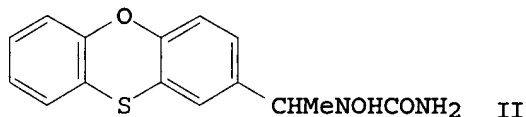
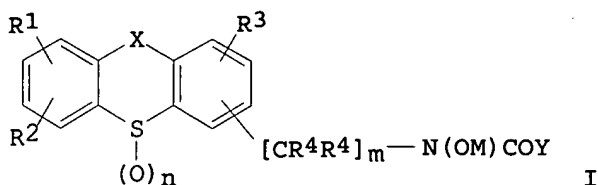
CODEN: USXXAM

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5036067	A	19910730	US 1990-493527	19900314 <--
	CA 2012137	AA	19910914	CA 1990-2012137	19900314 <--
	CA 2012137	C	20000808		
PRAI	US 1990-493527		19900314	<--	
OS	MARPAT 115:232258				
GI					



AB Title compds. I [R1-R3 = H, C1-7 alkyl, C1-7 alkoxy, C1-7 alkanoyloxy, CF3, cyano, NO2, OR4, NR4R4, NCOR4, SR5, SOR5, COR4, CO2R4, halo, etc.; R4 = H, C1-4 alkyl; R5 = C1-4 alkyl; R6 = H, C1-4 alkyl, COR4, etc.; R7 = H, C1-7 alkyl, Ar-substituted C1-7 alkyl; Ar = (substituted) Ph, furyl, or thienyl; X = X1, CH:CH, CH2CH2, CH2X1, X1CH2, NR7; X1 = O, S, SO, SO2, NR6; Y = R4, NR4R4; M = H, COAr, alkanoyl; m = 1-5; n = 0-2], useful for the treatment of **asthmatic**, inflammatory, or allergic conditions (no data), were prepared Thus, 2-acetylphenoxathiin was treated with NH2OH.HCl and the oxime formed was reduced by pyridine-borane to give 2-(1-hydroxaminoethyl)phenoxathiin. This was dissolved in THF and reacted with Me3SiNCO to give title compound II.

IC ICM A61K031-54

ICS A61K031-55; C07D279-18; C07D281-12

INCL 514224800

CC 28-12 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1

ST benzoheterocyclylhydroxamic acid prepn lipoxxygenase inhibitor;  
**antiasthmatic** benzoheterocyclylhydroxamic acid antiinflammatory  
 antiallergic; benzoheterocyclylhydroxy urea lipoxxygenase inhibitor; urea  
 benzoheterocyclylhydroxy **antiasthmatic** antiallergic  
 antiinflammatory

IT Bronchodilators

(**antiasthmetics**, dibenzoheterocyclylhydroxamic acids and  
 -hydroxy ureas)

IT 10274-08-5P 10318-51-1P, 2-Acetylphenoxathiin 10,10-dioxide  
 25324-52-1P, 2-Acetyl-10-methylphenothiazine 137131-81-8P 137131-82-9P  
 137131-83-0P, 2-Acetyl-8-bromophenoxathiin 137131-84-1P,  
 2-Acetyl-8-cyanophenoxathiin 137131-85-2P 137131-86-3P  
 137131-87-4P 137131-88-5P

RL: SPN (Synthetic preparation); **PREP (Preparation)**

(preparation of, as intermediate for lipoxxygenase inhibitors)

IT 137131-66-9P 137131-67-0P 137131-68-1P 137131-69-2P 137131-70-5P

137131-71-6P 137131-72-7P 137131-73-8P

137131-74-9P 137131-75-0P 137131-76-1P

137131-77-2P 137131-78-3P 137131-79-4P 137131-80-7P

137149-67-8P 137149-68-9P 137149-69-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)

(preparation of, as lipoxxygenase inhibitor)

IT 74-88-4, Methyl iodide, reactions 75-36-5, Acetyl chloride 334-88-3,  
 Diazomethane 544-92-3, Cuprous cyanide 874-87-3, 4-Methylthiobenzyl  
 chloride 917-54-4, Methyl lithium 1118-02-1, Trimethylsilyl isocyanate  
 5470-11-1, Hydroxylamine hydrochloride 5828-44-4, 2-Acetyl-8-

chlorophenothiazine 6631-94-3, 2-Acetylphenothiazine 7398-63-2  
 10230-35-0, 2-Bromophenoxathiin 10230-39-4, 2-Acetylphenoxathiin  
 10554-04-8 13229-20-4 40517-43-9, 4-Methylsulfonylbenzyl chloride  
 71474-60-7, Dibenzo[b,f]thiepin-3-carboxylic acid  
 71474-73-2 71475-19-9 71489-84-4 137131-89-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, in preparation of lipoxxygenase inhibitors)

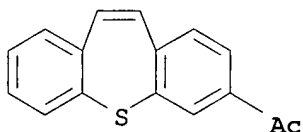
IT 137131-85-2P

RL: SPN (Synthetic preparation); PREP (Preparation); PREP  
 (Preparation)

(preparation of, as intermediate for lipoxxygenase inhibitors)

RN 137131-85-2 HCAPLUS

CN Ethanone, 1-dibenzo[b,f]thiepin-3-yl- (9CI) (CA INDEX NAME)



L26 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

AN 1991:492299 HCAPLUS

DN 115:92299

TI Preparation of [(dibenzo[b,f]thiepin-10-yl)piperazino]propylbenzimidazolones as antihistaminics and antianaphylactics

IN Jilek, Jiri; Protiva, Miroslav; Pomykacek, Josef; Metys, Jan Mudr;  
 Frycova, Hana

PA Czech.

SO Czech., 5 pp.

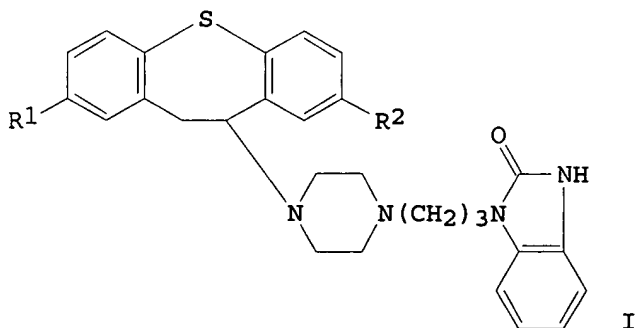
CODEN: CZXXA9

DT Patent

LA Czech

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CS 264934	B1	19890912	CS 1988-1524	19880309 <--
PRAI	CS 1988-1524		19880309	<--	
GI					



AB The title compds. (I; R1/R2 = H/H, H/Cl, Cl/H, H/SMe) and their hydrochloride salts were prepared by substitution reaction of the appropriate (dibenzo[b,f]thiepin-10-yl)piperazines with 1-(3-chloropropyl)-1,3-dihydro-2H-benzimidazol-2-one (II). To 50 mL PhMe were added (in order) 1-(10,11-dihydrodibenzo[b,f]thiepin-10-yl)piperazine 4.5, II 4.8, Et3N 2.3, and KI 0.15 g, and the mixture was refluxed 20 h to give 4.6 g title compound I (R1 = R2 = H) which was converted to its dihydrochloride salt (III). In a histamine aerosol test in guinea pigs the latter prevented bronchospasm with ED50 = 4.6 mg/kg p.o. In a passive cutaneous anaphylaxis test in rats, III had ED50 = 1.9 mg/kg p.o.

IC ICM C07D409-14

CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))  
Section cross-reference(s): 1

IT Bronchodilators  
(antiasthmatics, (dibenzothiepinyl)piperazino)propylbenzimidazolones)

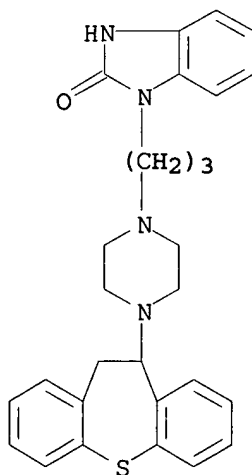
IT 121943-00-8P 121943-01-9P 121943-02-0P  
121943-03-1P 121943-04-2P 121943-05-3P  
121943-06-4P 121984-78-9P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as antianaphylactic and antihistaminic)

IT 4774-29-2 23048-89-7 27139-61-3  
52548-24-0  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(substitution reaction of, with (chloropropyl)dihydrobenzimidazolone, in preparation of antianaphylactic and antihistaminic)

IT 121943-00-8P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as antianaphylactic and antihistaminic)

RN 121943-00-8 HCAPLUS

CN 2H-Benzimidazol-2-one, 1-[3-[4-(10,11-dihydrodibenzo[b,f]thiepin-10-yl)-1-piperazinyl]propyl]-1,3-dihydro- (9CI) (CA INDEX NAME)



L26 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

AN 1986:68766 HCAPLUS

DN 104:68766

TI 6H-Dibenzo[b,f]thiepin compounds

IN Williams, Haydn; Rokach, Joshua

PA Merck Frosst Canada, Inc., Can.

SO Eur. Pat. Appl., 55 pp.

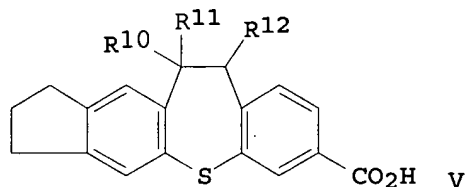
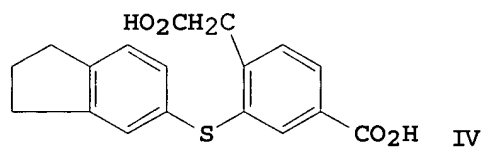
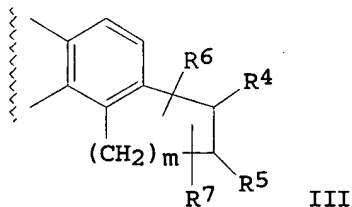
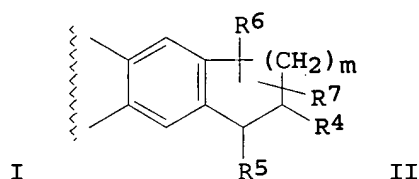
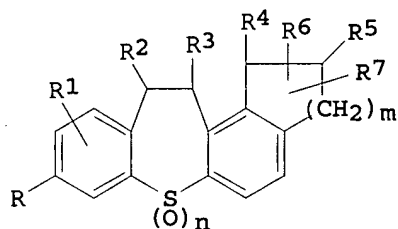
CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 138533	A2	19850424	EP 1984-306816	19841005 <--
	EP 138533	A3	19860122		
	EP 138533	B1	19890412		
	R: CH, DE, FR, GB, IT, LI, NL				
	US 4622403	A	19861111	US 1983-540480	19831011 <--
	CA 1245220	A1	19881122	CA 1984-465055	19841010 <--
	JP 60097976	A2	19850531	JP 1984-211560	19841011 <--
PRAI	US 1983-540480	A	19831011	<--	
OS	CASREACT 104:68766				
GI					

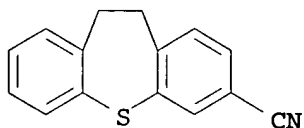


AB Dibenzo[b,f]thiepins I-III [R = 5-tetrazolyl, 5-tetrazolylmethyl, 3-hydroxy-1,2,5-thiadiazol-4-yl, 4-hydroxy-2,5-dioxo-Δ<sup>3</sup>-pyrrolin-3-yl, (CH<sub>2</sub>)<sub>x</sub>COR<sub>8</sub>, (un)masked CHO, (CH<sub>2</sub>)<sub>y</sub>OR<sub>9</sub>; R<sub>1</sub>, R<sub>6</sub>, R<sub>7</sub> = H, halogen, NO<sub>2</sub>, alkyl, (di)(alkyl)amino, alkanoyl, OH, alkoxy, acyloxy, alkylthio, CF<sub>3</sub>S, CF<sub>3</sub>, alkylsulfinyl, alkylsulfonyl; R<sub>6</sub>R<sub>7</sub> = O; R<sub>2</sub>-R<sub>5</sub> = H; R<sub>2</sub>R<sub>3</sub>, R<sub>4</sub>R<sub>5</sub> = bond; R<sub>8</sub> = OH, 2-imino-3-methylthiazolidine, (5-methyl-2-oxo-1,3-dioxolen-4-yl)methoxy, (un)substituted alkoxy, NH<sub>2</sub>; R<sub>9</sub> = H, alkylcarboxy, alkylcarboxamido, acyloxyalkyl, (un)substituted acyl; n = 0-2; m = 1, 2; x, y = 0-4] were prepared. Thus, 5-indanthiol and 4-carboxy-2-iodophenylacetic acid were refluxed with powdered Cu-KOH aqueous to give diacid IV, which was cyclized by CF<sub>3</sub>CO<sub>2</sub>H-(CF<sub>3</sub>CO)<sub>2</sub>O to give benzindenothiepin V.

(R10R11 = O, R12 = H). Reduction of the latter compound with NaBH<sub>4</sub> gave V (R10 = OH, R11 = R12 = H), which was dehydrated by H<sub>2</sub>SO<sub>4</sub>-AcOH to give V (R10R12 = bond, R11 = H). I are antagonists and biosynthesis inhibitors of contractile prostaglandins (no data).

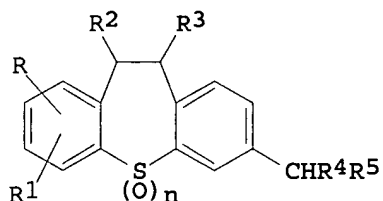
IC ICM C07D337-06  
ICS A61K031-38; C07D409-04; C07D337-14  
CC 27-21 (Heterocyclic Compounds (One Hetero Atom))  
ST dibenzothiepin; benzindenothiepin; prostaglandin inhibitor  
benzindenothiepin; antiallergic benzindenothiepin deriv;  
**antiasthmatic** benzindenothiepin deriv  
IT Bronchodilators and **Antiasthmatics**  
(benzindenothiepin derivs.)  
IT **71474-79-8**  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(formylation of)  
IT **99498-17-6P 99498-18-7P**  
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**  
(**Preparation**); RACT (Reactant or reagent)  
(preparation and alkylation by, of malonate)  
IT **99485-61-7P 99498-11-0P 99498-12-1P**  
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**  
(**Preparation**); RACT (Reactant or reagent)  
(preparation and borohydride reduction of)  
IT **99498-15-4P 99498-16-5P**  
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**  
(**Preparation**); RACT (Reactant or reagent)  
(preparation and bromination of)  
IT **99498-22-3P**  
RL: SPN (Synthetic preparation); **PREP** (**Preparation**)  
(preparation and conversion of, to acid chloride)  
IT **99498-07-4P 99498-08-5P 99498-19-8P 99498-20-1P**  
**99498-53-0P**  
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**  
(**Preparation**); RACT (Reactant or reagent)  
(preparation and hydrolysis of)  
IT **99485-58-2P 99498-21-2P 99498-24-5P**  
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**  
(**Preparation**); RACT (Reactant or reagent)  
(preparation and ring closure of)  
IT **99498-13-2P 99498-14-3P**  
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**  
(**Preparation**); RACT (Reactant or reagent)  
(preparation, hydrolysis, and decarboxylation of)  
IT **99498-09-6P 99498-10-9P**  
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**  
(**Preparation**); RACT (Reactant or reagent)  
(preparation, reduction, and condensation of, with malonate)  
IT **71474-79-8**  
RL: RCT (Reactant); **PREP** (**Preparation**); **PREP**  
(**Preparation**)  
(formylation of)  
RN **71474-79-8** HCAPLUS  
CN Dibenzo[b,f]thiepin-3-carbonitrile, 10,11-dihydro- (9CI) (CA INDEX NAME)



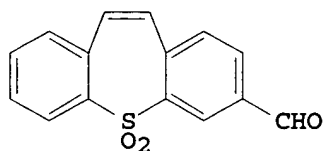


L26 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1985:596021 HCAPLUS  
 DN 103:196021  
 TI 3-Substituted dibenzo[b,f]thiepins and their use as prostaglandin antagonists  
 IN Rokach, Joshua  
 PA Merck Frosst Canada, Inc., Can.  
 SO Eur. Pat. Appl., 36 pp.  
 CODEN: EPXXDW  
 DT Patent  
 LA English  
 FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 138532	A2	19850424	EP 1984-306815	19841005 <--
	EP 138532	A3	19860212		
	R: CH, DE, FR, GB, IT, LI, NL				
	US 4535171	A	19850813	US 1983-540587	19831011 <--
	CA 1241007	A1	19880823	CA 1984-465056	19841010 <--
	JP 60115573	A2	19850622	JP 1984-211561	19841011 <--
PRAI	US 1983-540587	A	19831011	<--	
	US 1979-97759	A1	19791127	<--	
	US 1981-328096	A1	19810225	<--	
	US 1982-442921	A2	19821118	<--	
OS	CASREACT 103:196021; MARPAT 103:196021				
GI					



I



II

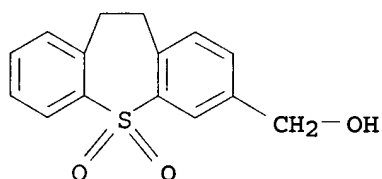
AB Dibenzothiepinicarboxaldehyde derivs. I [n = 0-2; R, R1 = H, halogen, alkyl, alkanoyl, OH, alkoxy, SH, alkylthio, alkylsulfinyl, alkylsulfonyl, CF3, CF3S, cyano, NO2, (di)(alkyl)amino, PhCH2, phenethyl, hydroxyalkyl; R2 = R3 = H, R2R3 = bond; R4, R5 = (di)(alkyl)amino, OH, SH, alkoxy, alkylthio; R4R5 = NR6, YXX1; R6 = H, alkyl, aryl, OH, alkoxy, acyloxy, (alkyl)amino; X, X1 = NR7, O, S; R7 = H, alkyl; Y = alkylene] were prepared. Thus, 3-cyanodibenzo[b,f]thiepin 5,5-dioxide was reduced by Raney alloy in aqueous HCO2H to give aldehyde II, which was converted to oximes, acetals and Schiff bases. I are prostaglandin antagonists, and are useful in treating a variety of conditions such as allergic asthma (no data).

IC ICM C07D337-14

ICS C07D409-04; A61K031-38

CC 27-21 (Heterocyclic Compounds (One Hetero Atom))

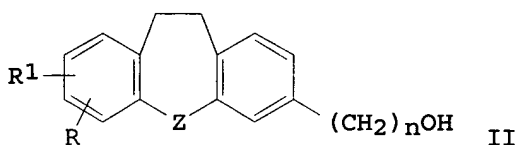
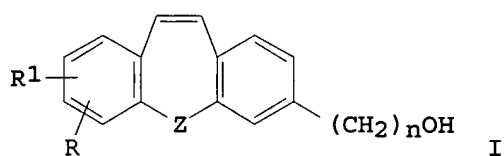
ST dibenzothiepinecarboxaldehyde prepn **antialsthmatic** prostaglandin  
antagonist; formyldibenzothiepin deriv  
IT Bronchodilators and **Antialsthmetics**  
(dibenzothiepinecarboxaldehyde derivs.)  
IT 77167-90-9 77167-92-1 77167-94-3  
77167-96-5 77167-97-6 77167-99-8  
77168-01-5 77168-02-6  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(oxidation of, to aldehyde)  
IT 99025-86-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**  
(**Preparation**); RACT (Reactant or reagent)  
(preparation and acetylation of)  
IT 79288-36-1P  
RL: SPN (Synthetic preparation); **PREP** (**Preparation**)  
(preparation and conversion of, to acetals, oximes, and Schiff bases)  
IT 79288-39-4P  
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**  
(**Preparation**); RACT (Reactant or reagent)  
(preparation and S-oxidation of)  
IT 79288-37-2P 79288-38-3P 79288-40-7P  
79288-41-8P 79288-42-9P 79288-43-0P  
79288-44-1P 79288-45-2P 79288-46-3P  
79288-47-4P 99025-87-3P 99025-88-4P  
99025-89-5P 99025-90-8P 99025-91-9P  
RL: SPN (Synthetic preparation); **PREP** (**Preparation**)  
(preparation of)  
IT 71474-59-4 71474-63-0 71474-79-8  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reduction of, to aldehyde)  
IT 77167-90-9  
RL: RCT (Reactant); **PREP** (**Preparation**); **PREP**  
(**Preparation**)  
(oxidation of, to aldehyde)  
RN 77167-90-9 HCAPLUS  
CN Dibenzo[b,f]thiepin-3-methanol, 10,11-dihydro-, 5,5-dioxide (9CI) (CA  
INDEX NAME)



L26 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN  
AN 1981:208728 HCAPLUS  
DN 94:208728  
TI 3-Hydroxymethyldibenzo[b,f]thiepins as prostaglandin antagonists  
IN Hamel, Pierre A.; Rokach, Joshua  
PA Merck Sharp and Dohme (I.A.) Corp., USA  
SO U.S., 13 pp.  
CODEN: USXXAM  
DT Patent  
LA English  
FAN.CNT 3  
PATENT NO. KIND DATE APPLICATION NO. DATE

KATHLEEN FULLER EIC1700 REMSEN 4B28 571/272-2505

PI	US 4237160	A	19801202	US 1979-97755	19791127 <--
	EP 29587	A1	19810603	EP 1980-107205	19801120 <--
	EP 29587	B1	19840613		
	R: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
	AT 7915	E	19840615	AT 1980-107205	19801120 <--
	ES 497132	A1	19821116	ES 1980-497132	19801125 <--
	DK 8005027	A	19810528	DK 1980-5027	19801126 <--
	JP 56099474	A2	19810810	JP 1980-165972	19801127 <--
	JP 02009591	B4	19900302		
PRAI	US 1979-97755	A	19791127	<--	
	US 1979-97759	A	19791127	<--	
	EP 1980-107205	A	19801120	<--	
GI					



AB Title compds. I and II [Z = S, S(O), SO<sub>2</sub>; n = 1, 2, 3, 4; R and/or R<sub>1</sub> is H, Cl, Br, F, iodo, NH<sub>2</sub>, alkyl, alkanoyl, OH, alkoxy, SH, alkylthio, alkylsulfinyl, alkylsulfonyl, CF<sub>3</sub>, SCF<sub>3</sub>, cyano, NO<sub>2</sub>, alkyl- or dialkylamino, aralkyl (e.g., PhCH<sub>2</sub> and PhCH<sub>2</sub>CH<sub>2</sub>), hydroxyalkyl, CH(OH)Me], useful in the treatment of allergic **asthma**, were prepared by different methods. Thus, dibenzo[b,f]thiepin-3-carboxylic acid was treated with B<sub>2</sub>H<sub>6</sub> in THF at room temperature to give I (Z = S, n = 1, R = R<sub>1</sub> = H) (III). The reaction of III with 3-ClC<sub>6</sub>H<sub>4</sub>C(O)OOH gave I [Z = S(O), n = 1, R = R<sub>1</sub> = H].

IC A61K031-38; C07D337-14

INCL 424275000

CC 27-22 (Heterocyclic Compounds (One Hetero Atom))

ST dibenzothiepinmethanol prepn allergic **asthma**;  
hydroxymethyldibenzothiepin prepn allergic **asthma**

IT **Asthma**

(allergic, (hydroxymethyl)dibenzothiepins for treatment of)

IT 77167-88-5P 77167-89-6P 77167-90-9P

77167-91-0P 77167-92-1P 77167-93-2P

77167-94-3P 77167-96-5P 77167-97-6P

77167-99-8P 77168-01-5P 77168-02-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

IT 71474-60-7 71474-64-1 71474-73-2

71474-76-5 77167-95-4 77167-98-7

77168-00-4 77168-03-7

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reduction of, by diborane)

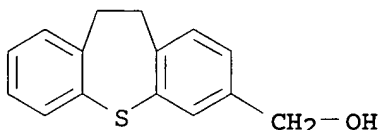
IT 77167-88-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 77167-88-5 HCAPLUS

CN Dibenzo[b,f]thiepin-3-methanol, 10,11-dihydro- (9CI) (CA INDEX NAME)



L26 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

AN 1979:540735 HCAPLUS

DN 91:140735

TI 10,11-Dihydro-11-oxodibenzo[b,f]thiepins

PA Merck and Co., Inc., USA

SO Jpn. Kokai Tokkyo Koho, 37 pp.

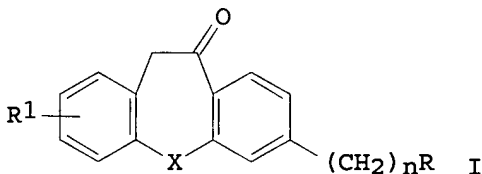
CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 54044692	A2	19790409	JP 1978-90550	19780726 <--
	EP 978	A1	19790307	EP 1978-300184	19780721 <--
	EP 978	B1	19820915		
	R: BE, CH, DE, FR, GB, LU, NL, SE				
	DK 7803306	A	19790127	DK 1978-3306	19780725 <--
	US 4394515	A	19830719	US 1981-251221	19810406 <--
PRAI	US 1977-819200	A	19770726	<--	
	US 1978-917211	A	19780623	<--	
OS	CASREACT 91:140735; MARPAT 91:140735				
GI					



AB Dihydroxodibenzothiepins I [X = S, SO, SO<sub>2</sub>; R = 5-tetrazolyl, 3-hydroxy-1,2,5-thiadiazol-4-yl, 4-hydroxy-2,5-dioxo-3-pyrrolin-3-yl, COR<sub>2</sub> (R<sub>2</sub> = OH, alkoxy, amino, etc.); n = 0-4; R<sub>1</sub> = H, halo, NH<sub>2</sub>, alkyl, alkanoyl, alkoxy, thiol, alkylamino, etc.] were prepared I are antagonists for prostaglandins and **asthma** (allergic) agents (no data). Thus, cyclization of 2-(3-BrC<sub>6</sub>H<sub>4</sub>S)C<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>COCl by AlCl<sub>3</sub> in (CH<sub>2</sub>Cl)<sub>2</sub> gave I (R = Br, n = 0, R' = H, X = S).

IC C07D337-14

CC 27-22 (Heterocyclic Compounds (One Hetero Atom))

ST prostaglandin antagonist dibenzothiepinone prepn; allergic **asthma** dibenzothiepinone; cyclization phenylthiophenylacetyl chlorideIT **Asthma**

(allergic, dibenzothiepinones in treatment of)

IT 71489-99-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and amidation of)

IT 71474-51-6P 71474-70-9P 71474-87-8P 71489-96-8P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and bromination of)

IT 71474-52-7P 71474-56-1P 71474-58-3P  
71474-78-7P 71474-88-9P 71474-94-7P  
71489-97-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and cyanation of)

IT 71474-82-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and cyclization of, with azide)

IT 71474-79-8P  
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and cyclization with azide)

IT 71490-08-9P  
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and cyclization with sulfur chloride)

IT 71474-57-2P 71474-93-6P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and dehydration of)

IT 71474-69-6P 71489-90-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and esterification of)

IT 71475-09-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and etherification of)

IT 71474-53-8P 71474-59-4P 71474-61-8P  
71474-63-0P 71474-68-5P 71474-72-1P  
71474-74-3P 71474-84-5P 71474-89-0P  
71474-95-8P 71474-98-1P 71475-00-8P  
71475-02-0P 71475-04-2P 71475-06-4P  
71475-18-8P 71489-83-3P 71489-86-6P  
71489-98-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and hydrolysis of)

IT 71474-66-3P 71474-73-2P 71474-80-1P  
71474-96-9P 71475-13-3P 71475-15-5P  
71475-19-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and oxidation of)

IT 71490-00-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and reaction of)

IT 71490-07-8P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and reaction with ammonia)

IT 71490-06-7P

RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**  
(**Preparation**); RACT (Reactant or reagent)  
(preparation and reaction with cyanide and ammonia)

IT 71474-68-5P  
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**  
(**Preparation**); RACT (Reactant or reagent)  
(preparation and reaction with formic acid and Raney nickel)

IT 71489-91-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**  
(**Preparation**); RACT (Reactant or reagent)  
(preparation and reaction with phosphoryl chloride)

IT 71475-10-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**  
(**Preparation**); RACT (Reactant or reagent)  
(preparation and reaction with thioxanthate)

IT 71489-85-5P  
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**  
(**Preparation**); RACT (Reactant or reagent)  
(preparation and rearrangement of)

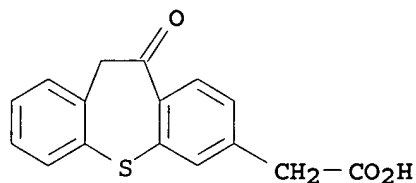
IT 20076-95-3P 20077-01-4P 25562-65-6P 71474-71-0P  
71474-77-6P 71474-92-5P  
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**  
(**Preparation**); RACT (Reactant or reagent)  
(preparation and reduction of)

IT 71474-60-7P 71474-62-9P 71474-64-1P  
71474-65-2P 71474-67-4P 71474-75-4P  
71474-76-5P 71474-81-2P 71474-83-4P  
71474-85-6P 71474-86-7P 71474-97-0P  
71474-99-2P 71475-01-9P 71475-03-1P  
71475-05-3P 71475-07-5P 71475-08-6P  
71475-11-1P 71475-12-2P 71475-14-4P  
71475-16-6P 71475-17-7P 71489-84-4P  
71489-87-7P 71489-88-8P 71489-89-9P  
71489-91-3P 71489-92-4P 71489-93-5P  
71489-94-6P 71489-95-7P 71490-01-2P  
71490-02-3P 71490-03-4P 71490-04-5P  
71490-05-6P 71490-09-0P 71490-10-3P  
71490-11-4P  
RL: SPN (Synthetic preparation); **PREP** (**Preparation**)  
(preparation of)

IT 71489-99-1P  
RL: RCT (Reactant); **PREP** (**Preparation**); **PREP**  
(**Preparation**); RACT (Reactant or reagent)  
(preparation and amidation of)

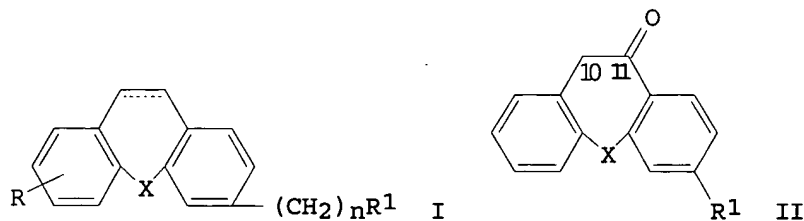
RN 71489-99-1 HCAPLUS

CN Dibenzo[b,f]thiepin-3-acetic acid, 10,11-dihydro-11-oxo- (9CI) (CA INDEX  
NAME)



AN 1979:540734 HCAPLUS  
 DN 91:140734  
 TI Dibenzo[b,f]thiepins  
 PA Merck and Co., Inc., USA  
 SO Jpn. Kokai Tokkyo Koho, 34 pp.  
 CODEN: JKXXAF  
 DT Patent  
 LA Japanese  
 FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 54044691	A2	19790409	JP 1978-90549	19780726 <--
	JP 62050470	B4	19871024		
	ES 471871	A1	19791001	ES 1978-471871	19780719 <--
	AU 7838177	A1	19800124	AU 1978-38177	19780719 <--
	AU 517813	B2	19810827		
	EP 11067	A1	19800528	EP 1978-300183	19780721 <--
	EP 11067	B1	19820421		
	R: BE, CH, DE, FR, GB, LU, NL, SE				
	NO 7802539	A	19790129	NO 1978-2539	19780724 <--
	DK 7803305	A	19790127	DK 1978-3305	19780725 <--
	FI 7802323	A	19790127	FI 1978-2323	19780725 <--
	ZA 7804231	A	19800227	ZA 1978-4231	19780725 <--
	DD 140746	C	19800326	DD 1978-206923	19780725 <--
	CA 1128048	A1	19820720	CA 1978-308068	19780725 <--
	PL 116355	B1	19810630	PL 1978-208653	19780726 <--
	PL 117756	B1	19810831	PL 1978-219619	19780726 <--
	PL 120813	B1	19820331	PL 1978-225727	19780726 <--
	ES 479215	A1	19790701	ES 1979-479215	19790402 <--
	ES 479216	A1	19790701	ES 1979-479216	19790402 <--
	ES 479217	A1	19790701	ES 1979-479217	19790402 <--
	ES 479218	A1	19791101	ES 1979-479218	19790402 <--
PRAI	US 1977-819199	A	19770726	<--	
	US 1978-917212	A	19780623	<--	
GI					



AB Dibenzotheiepins I [X = S, SO, SO<sub>2</sub>; R = H, halo, NH<sub>2</sub>, alkyl, alkanoyl, alkoxy, thiol, alkylamino etc.; n = 0-4; R<sub>1</sub> = 5-tetrazolyl, 3-hydroxy-1,2,5-thiadiazol-4-yl, 4-hydroxy-2,5-dioxo-3-pyrrolin-3-yl, COR<sub>2</sub> (R<sub>2</sub> = OH, alkoxy, amino, etc.)] were prepared I are antagonists of for prostaglandins and *antiasthma* agents. Thus, cyclization of 2-(3-BrC<sub>6</sub>H<sub>4</sub>S)C<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>COC1 by AlCl<sub>3</sub> in (ClCH<sub>2</sub>)<sub>2</sub> gave II (R<sub>1</sub> = Br, X = S), which was reduced by NaBH<sub>4</sub> to give the 11-OH derivative The latter was dehydrated by p-MeC<sub>6</sub>H<sub>4</sub>SO<sub>3</sub>H to give III (R<sub>1</sub> = Br, X = S), which was cyanated to give the 3-CN derivative (IV). Hydrolysis of IV gave III (R<sub>1</sub> = CO<sub>2</sub>H, X = S). Oxidation of IV by m-chloroperbenzoic acid gave sulfone III (R<sub>1</sub> = CN, X = SO<sub>2</sub>) (V). Hydrolysis of V gave III (R<sub>1</sub> = CO<sub>2</sub>H, X = SO<sub>2</sub>). Cyclization of V with NaN<sub>3</sub> gave III (R<sub>1</sub> = 5-tetrazolyl, X = SO<sub>2</sub>).

IC C07D337-14  
 CC 27-22 (Heterocyclic Compounds (One Hetero Atom))  
 ST prostaglandin antagonist dibenzothiepin prepn; allergic asthma  
 dibenzothiepin; cyclization phenylthiophenylacetyl chloride  
 IT **Asthma**  
 (allergic, dibenzothiepins in treatment of)  
 IT 71489-99-1  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (hydrolysis and oxidation by hydrogen peroxide)  
 IT 71474-51-6P 71474-70-9P 71489-96-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**  
 (**Preparation**); RACT (Reactant or reagent)  
 (preparation and bromination of, by phosphorus tribromide)  
 IT 71474-52-7P 71474-58-3P 71474-78-7P 71474-88-9P  
 71474-94-7P 71489-97-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**  
 (**Preparation**); RACT (Reactant or reagent)  
 (preparation and cyanation of)  
 IT 71474-82-3P  
 RL: SPN (Synthetic preparation); **PREP** (**Preparation**)  
 (preparation and cyclization with azide, tetrazole derivative from)  
 IT 71490-00-1P  
 RL: SPN (Synthetic preparation); **PREP** (**Preparation**)  
 (preparation and cyclization with di-Et oxalate, pyrroline derivative from)  
 IT 71490-08-9P  
 RL: SPN (Synthetic preparation); **PREP** (**Preparation**)  
 (preparation and cyclization with sulfur chloride, thiadiazole derivative  
 from)  
 IT 71474-71-0P  
 RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**  
 (**Preparation**); RACT (Reactant or reagent)  
 (preparation and debromination of)  
 IT 71474-57-2P 71474-93-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**  
 (**Preparation**); RACT (Reactant or reagent)  
 (preparation and dehydration of)  
 IT 71489-90-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**  
 (**Preparation**); RACT (Reactant or reagent)  
 (preparation and esterification and amidation of)  
 IT 71474-69-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**  
 (**Preparation**); RACT (Reactant or reagent)  
 (preparation and esterification of)  
 IT 71474-63-0P 71474-68-5P 71489-98-0P  
 RL: SPN (Synthetic preparation); **PREP** (**Preparation**)  
 (preparation and hydrolysis and cyclization with azide)  
 IT 71475-02-0P  
 RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**  
 (**Preparation**); RACT (Reactant or reagent)  
 (preparation and hydrolysis and diazotization of)  
 IT 71474-72-1P 71474-95-8P 71475-04-2P  
 71475-18-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**  
 (**Preparation**); RACT (Reactant or reagent)  
 (preparation and hydrolysis and oxidation of)  
 IT 71474-53-8P 71474-61-8P 71474-74-3P  
 71474-84-5P 71474-89-0P 71474-98-1P  
 71475-00-8P 71475-06-4P 71489-83-3P  
 71489-86-6P



RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and hydrolysis of)

IT 71474-79-8P  
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and oxidation and cyclization with azide)

IT 71474-73-2P 71475-15-5P  
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and oxidation by hydrogen peroxide)

IT 71474-66-3P  
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and oxidation by peroxide, S-oxide from)

IT 71474-62-9P 71474-96-9P 71475-13-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and oxidation of)

IT 71474-80-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and oxidation of, S-oxide from)

IT 71475-19-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and oximation and oxidation of)

IT 71474-59-4P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and reaction of)

IT 71490-07-8P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and reaction with ammonia)

IT 71474-68-5P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and reaction with formic acid and Raney nickel, aldehyde from)

IT 71489-91-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and reaction with phosphoryl chloride)

IT 71490-06-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and reaction with sodium cyanide and ammonia)

IT 71475-10-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and reaction with thioxanthate)

IT 71489-85-5P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and rearrangement of)

IT 20076-95-3P 20077-01-4P 25562-65-6P 71474-56-1P 71474-77-6P 71474-92-5P 71474-99-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and reduction of)

IT 71475-09-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

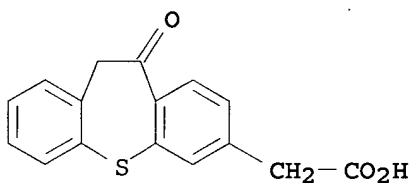
(preparation and O-methylation of)

IT 71474-60-7P 71474-64-1P 71474-65-2P  
71474-67-4P 71474-75-4P 71474-76-5P  
71474-81-2P 71474-83-4P 71474-85-6P  
71474-86-7P 71474-97-0P 71475-01-9P  
71475-03-1P 71475-05-3P 71475-07-5P  
71475-08-6P 71475-11-1P 71475-12-2P  
71475-14-4P 71475-16-6P 71475-17-7P  
71489-84-4P 71489-87-7P 71489-88-8P  
71489-89-9P 71489-91-3P 71489-92-4P  
71489-93-5P 71489-94-6P 71489-95-7P  
71490-01-2P 71490-02-3P 71490-03-4P  
71490-04-5P 71490-05-6P 71490-09-0P  
71490-10-3P 71490-11-4P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

IT 71489-99-1  
RL: RCT (Reactant); PREP (Preparation); PREP  
(Preparation)  
(hydrolysis and oxidation by hydrogen peroxide)

RN 71489-99-1 HCAPLUS

CN Dibenzo[b,f]thiepin-3-acetic acid, 10,11-dihydro-11-oxo- (9CI) (CA INDEX NAME)



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